Functional determinants via Wronski construction of Green functions

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A general technique is developed for calculating functional determinants of second-order differential operators with Dirichlet, periodic, and antiperiodic boundary conditions. As an example, we give simple formulas for a harmonic oscillator with an arbitrary time-dependent frequency. Here our result is a generalization of Gel'fand-Yaglom's famous formula which was restricted to Dirichlet boundary conditions. Apart from the generalization, our derivation is more transparent than theirs, the determinants requiring only knowledge of the classical trajectories. Special properties of operators with a zero mode are exhibited. Our technique does not require the calculation of the spectrum and is as simple as Wronski's method for Green functions.

1. Evaluation of Gaussian path integrals is necessary in many physical problems. In particular, it appears in all semi-classical calculations of fluctuating systems. Typically, it leads to the problem of calculating the functional determinant of a second-order differential operator [1]. For Dirichlet boundary conditions, a first general solution of this problem was given by Gel'fand and Yaglom [2] based on the lattice approximation to path integrals in the continuum limit. Their result was expressed in terms of a simple differential equation for the functional determinant. In subsequent work [3]– [6], the formalism was generalized to a variety of differential operators and boundary conditions based on the concept of zeta-function regularization [7]. Unfortunately, Gel'fand-Yaglom's method becomes rather complicated for periodic and antiperiodic boundary condition relevant in quantum statistic (see Section 2.12 in [1]). In the periodic case there is, moreover, a zero mode causing additional complications.

In this paper we present a systematic method for finding functional determinants of linear differential operators which is based on Wronski's simple construction of Green functions. Our method is simpler than those used in the previous approaches, since the determinants are expressed entirely in terms of a classical trajectory. Furthermore, for fluctuation operator with a zero mode, a case frequently encountered in semiclassical calculations, the special treatment of this mode becomes transparent.

2. The typical fluctuation action arising in semiclassical approximations has a quadratic Lagrangian of the form

$$L = \frac{M}{2}\left[\dot{x}^2 - \Omega^2(t)x^2\right]. \tag{1}$$

Physically, this Lagrangian describes a harmonic oscillator with a time-dependent frequency $\Omega(t)$. The path integral for such a system was studied in several papers [8]– [11]. For such an oscillator, both the quantum mechanical propagator and the thermal partition function contain a phase factor $\exp[iS_{\mathrm{cl}}(x)]$ and are multiplied by a pre-exponential fluctuation factor proportional to

$$F(t_b, t_a) \sim \left(\frac{\mathrm{Det}K_1}{\mathrm{Det}\tilde{K}}\right)^{-1/2}, \tag{2}$$

where $K_1 = -\partial_t^2 - \Omega^2(t) \equiv K_0 - \Omega^2(t)$ is the kernel of the second variation of action $S(x)$ along the classical path $x_{\mathrm{cl}}(t)$. The linear operator K_1 acts on the space of twice differentiable functions $y(t) = \delta x(t)$ on an interval $t \in [t_a, t_b]$ with appropriate boundary conditions. These are Dirichlet boundary conditions $y(t_a) = y(t_b) = 0$ in the quantum-mechanical case, and periodic (antiperiodic) $y(t_b) = \pm y(t_a), \dot{y}(t_b) = \pm \dot{y}(t_a)$ in the quantum statistical case. In these two cases the operator $\tilde{K}$ may be chosen as K_0 or $K_0 - \omega_0^2$, respectively, where ω_0 is a time-independent oscillator frequency. The ratio of determinants (2) arises naturally from the normalization of the path integral and is well-defined [1]. Furthermore, for such an operator we may assume the Fredholm property

$$\frac{\mathrm{Det}K_1}{\mathrm{Det}\tilde{K}} = \mathrm{Det}\tilde{K}^{-1}K_1 \tag{3}$$

thus neglecting multiplicative anomalies [12]. Since the operator $\tilde{K}^{-1}K_1$ is of the form $I+B$, with B an operator of the trace class, it has a well-defined determinant even without any regularization.

To calculate $F(t_b, t_a)$, we introduce a one-parameter family of operators K_g depending linearly on the parameter $g : K_g = K_0 - g\Omega^2(t), 0 \ll g \ll 1$. The above property (3) allows us to make use of the well-known formula $\log \mathrm{Det}\tilde{K}^{-1}K_g = \mathrm{Tr} \log \tilde{K}^{-1}K_g$ to relate the g-derivative of the logarithm of the ratio (2) to the trace of the Green function of the operator K_g as follows

$$\partial_g \log \mathrm{Det}\tilde{K}^{-1}K_g = -\mathrm{Tr}\, \Omega^2(t)G_g(t,t'), \tag{4}$$

the Green function being defined by

$$G_g(t,t') = [-\partial_t^2 - g\Omega^2(t)]^{-1}\delta(t-t'). \tag{5}$$

Formula (4) is valid provided we regularize the trace on the right-hand side, if it diverges, via zeta-functions

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$\zeta(s) = \sum_i \lambda^{-s}$, where the sum runs over all eigenvalues. It is convergent for sufficinetly large s and defined for smaller s by analytic continuation (see [7]). Then, for each member of the g-family, $\mathrm{Det}K_1 = \exp[-\xi'(0)]$. Another proof of (4) can be found in [3].

By integrating (4), we obtain for the ratio of functional determinants (3):

$$\mathrm{Det}\tilde{K}^{-1}K_g = C \exp\left\{ -\int_0^g dg' \int_{t_a}^{t_b} dt\, \Omega^2(t) G_{g'}(t,t) \right\},$$
(6)

where $C = \mathrm{Det}\tilde{K}^{-1}K_0$ is a g-independent constant. This is our basic formula to be supplemented by an appropriate boundary condition to Eq. (5) for the Green function as we shall now discuss in detail.

3. A general solution of Eq. (5) is given by advanced or retarded Green functions as follows

$$G_g^-(t,t') = G_g^+(t',t) = \Theta_{tt'} \cdot f_g(t,t'),$$
(7)

where $\Theta_{tt'} = \Theta(t-t')$ is Heaviside's function and $f_g(t,t')$ is a combination

$$f_g(t,t') = \frac{1}{W_g}\left[\eta_g(t)\xi_g(t') - \xi_g(t)\eta_g(t')\right]$$
(8)

of two linearly independent solutions $\eta_g(t)$ and $\xi_g(t)$ of the homogeneous equation

$$\left[-\partial_t^2 - g\Omega^2(t)\right]h_g(t) = 0.$$
(9)

The constant W_g is the time independent Wronski determinant $W_g = \eta_g \dot{\xi}_g - \dot{\eta}_g \xi_g$. The solution (7) is not unique since it leaves room for an additional general solution of the homogeneous equation (9) with an arbitrary coefficients. This freedom is removed by appropriate boundary conditions. Consider first the quantum mechanical case which requires Dirichlet boundary conditions $y(t_b) = y(t_a) = 0$ for the eigenfunctions $y(t)$ of K_1, implying for the Green function the boundary conditions

$$G_g(t_a,t') = 0, \quad t \leq t'.$$
$$G_g(t',t_b) = 0, \quad t' \leq t.$$
(10)

The operator $\tilde{K}$ in the ratio (2) is equal to K_0, and the constant C in Eq. (6) is unity. After imposing (10), the Green function is uniquely given by Wronski's formula:

$$G_g(t,t') = \frac{\Theta_{tt'}f_g(t',t_a)f_g(t_b,t) + \Theta_{t't}f_g(t,t_a)f_g(t_b,t')}{f_g(t_a,t_b)},$$
(11)

where

$$f_g(t_a,t_b) = \frac{\mathrm{Det}\Lambda_g}{W_g} \neq 0,$$
(12)

with Λ being a constant (2×2)-matrix

$$\Lambda = \begin{pmatrix} \eta_a & \xi_a \\ \eta_b & \xi_b \end{pmatrix},$$
(13)

formed from the solutions $\eta_g(t)$ and $\xi_g(t)$ at arbitrary $g \neq 1$. Note that these solutions are restricted only the condition (12). The result is unique and well-defined, assuming the absence of a zero mode $\xi(t)$ of the operator K_1 with Dirichlet boundary conditions $\xi_a = \xi_b = 0$. Such a mode would cause problems since according to (10), the Wronski determinant W would vanish at the initial point, and thus for all t.

Excluding zero modes, we obtain from (8):

$$\mathrm{Tr}\,\Omega^2(t)G_g(t,t') = \frac{1}{f_g(t_a,t_b)}\int_{t_a}^{t_b} dt\, \Omega^2(t) f_g(t,t_a) f_g(t_b,t).$$
(14)

To perform the time integral on the right hand side, we make use of the identity

$$\Omega^2(t)\xi(t)\eta(t) = \partial_t[\dot{\eta}_g(t)\partial_g \xi_g(t) - \eta_g(t)\partial_g \dot{\xi}_g(t)].$$
(15)

This follows from Eq. (9) for $\eta(t,g)$, and an analogous equation for $\xi_{\tilde{g}}(t)$, after multiplying the first by $\xi_{\tilde{g}}(t)$ and the second by $\eta_g(t)$, and taking their difference. In the limit $\tilde{g} \to g$, we obtain (15) from the linear term in $\tilde{g} - g$. Inserting (15) into (14), we see that

$$\mathrm{Tr}\,\Omega^2(t)G_g(t,t') = -\partial_g \log\left(\frac{\mathrm{Det}\Lambda_g}{W_g}\right).$$
(16)

Substituting (16) into (6), we find

$$\mathrm{Det}K_0^{-1}K_g = \frac{\mathrm{Det}\Lambda_g}{W_g}\bigg/\frac{\mathrm{Det}\Lambda_0}{W_0},$$
(17)

where $\mathrm{Det}\Lambda_0/W_0 = t_b - t_a$. Finally, setting to $g = 1$ in (17) gives the required ratio of the functional determinants

$$\mathrm{Det}K_0^{-1}\cdot K_1 = \frac{\mathrm{Det}\Lambda_g}{W_g}\bigg/(t_b - t_a).$$
(18)

In a time-sliced quantum mechanical path integral, the determinant of K_0 is finite and has the value [1]

$$\mathrm{Det}K_0 = t_b - t_a,$$
(19)

so that we obtain

$$\mathrm{Det}K_1 = \frac{[\eta_1(t_a)\xi_1(t_b) - \eta_1(t_b)\xi_1(t_a)]}{W_1},$$
(20)

which coincides with Gel'fand-Yaglom's formula (see Section 2.7 in [1]).

For a harmonic oscillator with a time-dependent frequency $\Omega(t)$ it is convenient to relate the set of two independent solutions $\eta_g(t)$ and $\xi_g(t)$ of Eq. (9) at $g = 1$,

for which we omit the subscripts g, to the classical path $x_{\rm cl}(t) = x_a\xi(t) + x_b\eta(t)$ satisfying the endpoint conditions $x_{\rm cl}(t_a) = x_a$ and $x_{\rm cl}(t_b) = x_b$. Since this construction satisfies $\eta_a = \xi_b = 0$, $\eta_b = \xi_a = 1$ and $W = \dot{\xi}_b = -\dot{\eta}_a$, the explicit solution being

$$\xi(t) = \frac{\partial x_{\rm cl}(t)}{\partial x_a} = \frac{p(t)p_b \sin\omega_0(q_b - q)}{p_a p_b \sin\omega_0(q_b - q_a)},$$
$$\eta(t) = \frac{\partial x_{\rm cl}(t)}{\partial x_b} = \frac{p(t)p_a \sin\omega_0(q - q_a)}{p_a p_b \sin\omega_0(q_b - q_a)}, \tag{21}$$

They are parametrized by two functions $q(t)$ and $p(t)$ satisfying the constraint

$$\omega_0 \dot{q} p^2 = 1, \tag{22}$$

where ω_0 is an arbitrary constant frequency. The function $p(t)$ satisfies the Ermakov-Pinney equation [13]

$$\ddot{p} + \Omega^2(t)p - p^{-3} = 0. \tag{23}$$

Inserting (21) into (18), we obtain for the harmonic oscillator with a time-dependent frequency $\Omega(t)$ the ratio of functional determinants

$$\mathrm{Det}K_0^{-1}K_1 = \frac{p_a p_b \sin\omega_0(q_b - q_a)}{(t_b - t_a)}. \tag{24}$$

where subscripts a and b indicate avaluation at $t = t_a$ and $t = t_b$, respectively. We check this representation by expressing the right-hand side in terms of the classical action $S_{\rm cl}(x)$. With the same normalization as in (19), this yields the well-known one-dimensional Van-Vleck formula

$$\mathrm{Det}K_1 = -M[\partial^2 S_{\rm cl}(x_a, x_b)/\partial x_a \partial x_b]^{-1} \tag{25}$$

To end this section we note that the ratio (18) can easily be extended to the stochastic case where the final position of the trajectory $x(t)$ remains unspecified. To this end we consider Eqs. (14) and (15) with a variable upper time $t' \geq t \geq t_a$. Then the eigenvalues of the operator $K_0^{-1}K_1$ become functions of t' with a phase factor produced by each passage through a focal point.

4. Consider now periodic (antiperiodic) boundary conditions $y(t_b) = \pm y(t_a)$, $\dot{y}(t_b) = \pm\dot{y}(t_a)$ for the eigenfunctions $y(t)$ of the operator K_1 and the for Green function $G^{\,p}_{\,a}(t,t')$:

$$G^{\,p}_{\,a}(t_b, t') = \pm G^{\,p}_{\,a}(t_a, t'),$$
$$\dot{G}^{\,p}_{\,a}(t_b, t') = \pm\dot{G}^{\,p}_{\,a}(t_a, t'), \tag{26}$$

where $T = t_b - t_a$ is the period. In both cases, the frequency $\Omega(t)$ and Dirac's δ-function in Eq. (5) are also assumed to be periodic (antiperiodic) with the same period. The general solution of Eq. (5) satisfying the boundary

conditions (26) is constructed by adding to (7) an expression of the same type as before, using the same homogeneous solutions $\eta_g(t)$ and $\xi_g(t)$. The result has the form

$$G^{\,p}_{\,a\,g}(t,t') = G_g(t,t')$$
$$\mp \frac{[f_g(t,t_a) \pm f_g(t_b,t)][f_g(t',t_a) \pm f_g(t_b,t')]}{\Delta^{\,p}_{\,a} \cdot f_g(t_a,t_b)} \tag{27}$$

with the condition

$$\Delta^{\,p}_{\,a} = \frac{\mathrm{Det}\bar{\Lambda}^{\,p}_{\,a\,g}}{W_g} \neq 0, \tag{28}$$

where $\bar{\Lambda}^{\,p}_{\,a}$ are now the (2×2)-constant matrices

$$\bar{\Lambda}^{\,p}_{\,a} = \begin{pmatrix} (\eta_b \mp \eta_a) & (\xi_b \mp \xi_a) \\ (\dot{\eta}_b \pm \dot{\eta}_a) & (\dot{\xi}_b \mp \dot{\xi}_a), \end{pmatrix} \tag{29}$$

evaluated at $g \neq 1$. In analogy to Eq. (16) we now find the formula

$$\mathrm{Tr}\,\Omega^2(t)G^{\,p}_{\,a\,g}(t,t') = -\partial_g \log\left(\frac{\mathrm{Det}\bar{\Lambda}^{\,p}_{\,a\,g}}{W_g}\right). \tag{30}$$

Substituting this into (6) and setting $g = 1$, we obtain the ratio of the functional determinants for periodic boundary conditions

$$\mathrm{Det}\tilde{K}^{-1} \cdot K_1 = \frac{\mathrm{Det}\Lambda^{p}_1}{W_1} \Big/ 4\sin^2\frac{\omega_0(t_b - t_a)}{2} \tag{31}$$

Here $\mathrm{Det}\,\tilde{K} = \mathrm{Det}(-\partial_t^2 - \omega_0^2)$ is the fluctuation determinant of the harmonic oscillator, which in the same normalization as in (19) is equal to

$$\mathrm{Det}\,\tilde{K} = 4\sin^2\frac{\omega_0(t_b - t_a)}{2}, \tag{32}$$

and thus the formula

$$\mathrm{Det}K_1 = \frac{(\eta_b - \eta_a)(\dot{\xi}_b - \dot{\xi}_a) - (\xi_b - \xi_a)(\dot{\eta}_b - \dot{\eta}_a)}{W}, \tag{33}$$

the right-hand side being evaluated at $g = 1$. For antiperiodic boundary conditions, the analogous expressions are

$$\mathrm{Det}\tilde{K}_1^{-1} = \frac{\mathrm{Det}\Lambda^{a}_1}{W_1} \Big/ 4\cos^2\frac{\omega_0(t_b - t_a)}{2}, \tag{34}$$

$$\mathrm{Det}K_1 = \frac{(\eta_b + \eta_a)(\dot{\xi}_b + \dot{\xi}_a) - (\xi_b + \xi_a)(\dot{\eta}_b + \dot{\eta}_a)}{W}. \tag{35}$$

For a harmonic oscillator with a time-dependent frequency $\Omega(t)$, we use again the representation (21) for $\xi(t)$ and $\eta(t)$ in terms of the functions $p(t)$ and $q(t)$, which in

addition to (22) and (23) have the following properties: the function $p(t)$ is periodic and even

$$p(t+T) = p(t), \quad p(-t) = p(t) \qquad (36)$$

so that $p_b = p_a$, whereas the function $q(t)$ satisfies

$$q(t+T) = q(t) + q_b, \quad q_a = 0, \qquad (37)$$

where $T \equiv (t_b - t_a)$. Inserting now the solutions (21) into (31) and (34), we find the ratio of functional determinants for a harmonic oscillator with a time-dependent frequency $\Omega(t)$ with periodic boundary conditions

$$\mathrm{Det}\,\tilde{K}^{-1}K_1 = 4\sin^2\frac{\omega_0 q_b}{2}\Big/4\sin^2\frac{\omega_0 t}{2}, \qquad (38)$$

and with antiperiodic boundary conditions

$$\mathrm{Det}\,\tilde{K}^{-1}K_1 = 4\cos^2\frac{\omega_0 q_b}{2}\Big/4\cos^2\frac{\omega_0 t}{2}. \qquad (39)$$

Note that only formula (24) for the Dirichlet boundary condition has been known in the literature (see [8]– [11]). The periodic and antiperiodic formulas (38) and (39) are new, although they have had predecssors on the lattice [15]. Moreover, our new derivation has the advantage of employing only Wronski's simple construction method for Green functions. The general expressions for the functional determinants (20), (33) and (35) are form-invariant under an arbitrary changes $(\eta, \xi) \to (\tilde{\eta}, \tilde{\xi})$ of the basic set $\eta(t)$ and $\xi(t)$ of two independent solutions of the homogeneous equation (9).

5.   Contrary to the case of a harmonic oscillator with a time-dependent frequency $\Omega(t)$, consider now the situation where the operator K_1 has a zero mode. In this case we may assume the frequency $\Omega(t)$ in Eq. (1) the special form $\Omega^2(t) = V''(x_{\mathrm{cl}}(t))/M$ with a potential $V(x)$, allowing reflecting the translation invariance of the theory with Lagrangian (1) along the time axis [16]. Let $\xi(t)$ be the corresponding eigenfunction satisfy the condition $\xi_a = 0$ as well as $\xi_b = 0$. As mentioned above, the condition (12) is now violated, making Eq. (11) undefined, and it is impossible to construct two independent solution $\xi(t)$ and $\eta(t)$ since their Wronski determinant would be equal to zero indentically $W = \eta_a\dot{\xi}_a - \dot{\eta}_a\xi_a \equiv 0$ due to the boundary conditions (10). Since the Wronski construction is not applicable we replace

$$\xi_b = 0, \quad \xi_a = 0 \qquad (40)$$

by the regularized conditions

$$\xi_b^{\varepsilon} = 0, \quad \xi_a^{\varepsilon} = \varepsilon. \qquad (41)$$

These do not require a new calculation of the determinant (20), and we find immediately

$$\mathrm{Det}\,K_1^{\varepsilon} = -\frac{\varepsilon}{\dot{\xi}_b} \to 0, \qquad (42)$$

in the limit $\varepsilon \to 0$. We therefore remove the zero mode from the determinant using the standard method [17]. The regularized determinant is defined by

$$\mathrm{Det}\,K_1^R = \lim_{\varepsilon \to 0}\frac{\mathrm{Det}\,K_1^{\varepsilon}}{\lambda^{\varepsilon}}, \qquad (43)$$

where λ^{ε} is the eigenvalue associated with the eigenfunction $\xi^{\varepsilon}(t)$.

$$K_1\xi^{\varepsilon} = \lambda^{\varepsilon}\xi^{\varepsilon}, \qquad (44)$$

with the limits $\xi^{\varepsilon} \to \xi$, $\lambda^{\varepsilon} \to 0$ for $\varepsilon \to 0$. To first order in ε it follows from (44) that

$$\int_{t_a}^{t_b} dt\,\xi K_1\xi^{\varepsilon} \approx \lambda^{\varepsilon}\int_{t_a}^{t_b} dt\,\xi^2(t) \equiv \lambda^{\varepsilon}\langle \xi|\xi\rangle. \qquad (45)$$

Integrating the left-hand side by parts and taking into account the conditions (40) and (41) gives

$$\lambda^{\varepsilon} = -\varepsilon\frac{\dot{\xi}_a}{\langle \xi|\xi\rangle}. \qquad (46)$$

Finally, substituting (46) and (42) into (43) we obtain the functional determinant without zero mode

$$\mathrm{Det}\,K_1^R = \frac{<\xi|\xi>}{\dot{\xi}_a\dot{\xi}_b}. \qquad (47)$$

For periodic (antiperiodic) boundary conditions $y(t_a) = \pm y(t_b), \dot{y}(t_a) = \pm\dot{y}(t_b)$, the analogous formula is

$$\mathrm{Det}\,K_1^R = \frac{(\xi_b \mp \xi_a)<\xi|\xi>}{\eta_a(\eta_a\dot{\xi}_a - \dot{\eta}_a\xi_b)}. \qquad (48)$$

In the periodic case, formula (48) is useful for semiclassical calculations of path integrals processing nontrivial classical solutions such as solitons or instantons [1].

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